

# Simulation of Injection Molding Thermoplastic Reinforced with Micro and Nano-Particles

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# ABSTRACT

The redefinitions of the energy policy of the US have multiple fronts. One objective of the DOE is to enforce the development of new lightweight materials with identical or better properties than existing materials. The goal is to reduce the weight of vehicles by 33% (in comparison to 2002) by 2010. One of the promising alternatives under consideration is injection molded parts made of polymers reinforced with large aspect ratio particles (i.e. long fibers or nanoparticles). However, these types of parts have not been successfully manufactured because of the unknown molecular behavior of the materials during processing. In this research we are trying to extend the Doi's theory for rod-like systems to simulate the rheological behavior of these composites.

A numerical code is being written to simulate the flow of fiber suspensions in injection molding flow geometries. The preliminary results of the simulation for shear flow shows that the model can reproduce the experimental data under stress growth conditions. The code has been validated in shear and extensional flow which are used to determine material parameters.

# BACKGROUND

## High Strength Weight Reduction Materials

Office of FreedomCAR and Vehicle Technologies



To identify and develop materials and **materials processing technologies** which can contribute to weight reduction without sacrificing strength and functionality:

- Increase the fuel efficiency
- Reduce emissions of class 1-8 trucks

## GOAL

To combine numerical simulation and experimental programs to confirm the prediction of microstructure in both glass and nano-particle reinforced thermoplastics

# OBJECTIVES

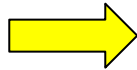
- To simulate the mold filling process for thermoplastic melts reinforced with short fibers, long fibers and nano-particles of high aspect ratio using constitutive relations (i.e. stress tensors coupled with a generation expression) which allow coupling between the flow and particle orientation.
- A key aspect of this work will be an experimental evaluation of the predicted fiber or particle orientation distribution throughout an injection molded part.

# INNOVATION

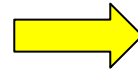
Use of **constitutive relations**, which contain the **micro-structural aspects** of the reinforced melts and **viscoelastic effects**.

# ORIENTATION DURING INJECTION MOLDING

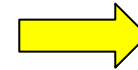
Phase I:  
Plastification



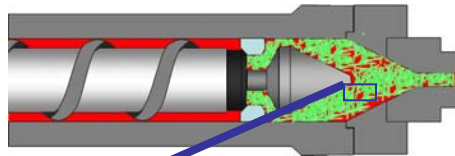
Phase II:  
Filling



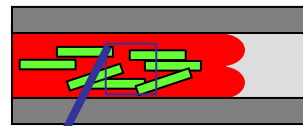
Phase III:  
Packing



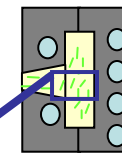
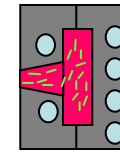
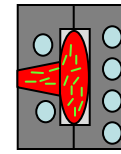
Phase IV:  
Cooling



Random orientation in the tip of screw

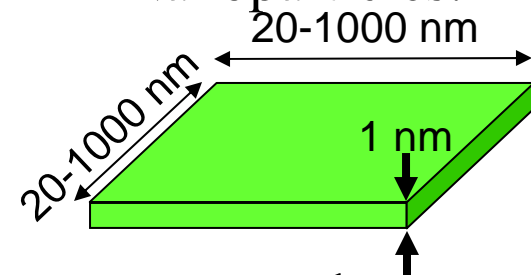


Orientation when flowing in the mold and runner



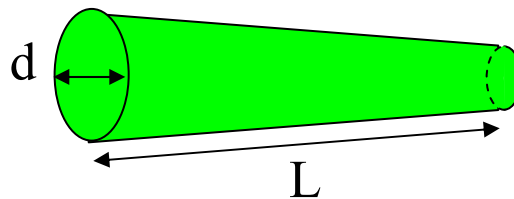
Loose orientation as part is packed or cooled

Nanoparticles:



Nanoclays  
(i.e. Montmorillenite)

Fibers:

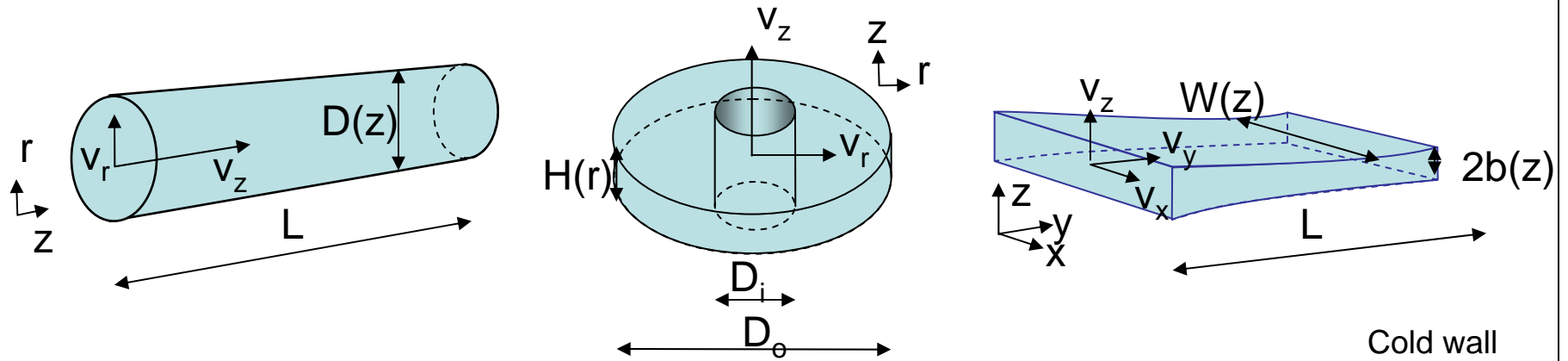


Long fiber:  $AR \leq 1$

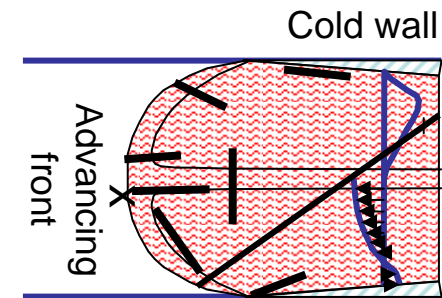
Short fiber:  $AR > 1$

$$\text{Aspect Ratio} = \frac{\text{Length}}{\text{Diameter}}$$

## Geometric elements commonly found in injection molding tooling



- Mechanism of flow  
Shear and Elongational flow



## CHALLENGES

- **Predict fiber orientation correctly: Should Doi Model be improved**
- **Develop a stable and accurate numerical scheme**
- **To measure fiber orientation**
- **Is the final flow induced orientation governed by the Brownian motion effects or by the relaxation process of the system, *i.e.* elastic recoiling of non-Newtonian matrix?**

# MODELLING

➤ Behavior of polymer-glass fiber:

➤ Actual model: Doi Theory: LCP assuming Newtonian solvent

*Evolution tensor of orientation*

$$\frac{\partial \underline{\underline{S}}}{\partial t} = \underline{\underline{F}}(\underline{\underline{S}}) + \underline{\underline{G}}(\underline{\underline{S}})$$

*Brownian contribution*

$$\underline{\underline{F}}(\underline{\underline{S}}) = -6\overline{D}_r \left( \underline{\underline{A}} - \frac{1}{3}\underline{\underline{I}} \right) + 6\overline{D}_r U \left( \underline{\underline{S}} \bullet \underline{\underline{S}} - \underline{\underline{S}} \bullet \underline{\underline{S}} \underline{\underline{S}} \right)$$

*Kinematics contribution*

$$\underline{\underline{G}}(\underline{\underline{S}}) = (\underline{\underline{\nabla v}})^T \bullet \underline{\underline{S}} + \underline{\underline{S}} \bullet \underline{\underline{\nabla v}} - 2 \left( \underline{\underline{\nabla v}} + (\underline{\underline{\nabla v}})^T \right) : \underline{\underline{S}} \underline{\underline{S}}$$

*Stress due oriented fiber*

$$\underline{\underline{\tau}} = \underbrace{G \left[ \underline{\underline{S}} - \frac{1}{3}\underline{\underline{I}} - U \underline{\underline{S}} \bullet \underline{\underline{S}} + U \underline{\underline{S}} : \underline{\underline{S}} \underline{\underline{S}} \right]}_{\text{Original Doi Theory stress equation}} + \underbrace{\frac{AG}{6D_r} \left[ \underline{\underline{\nabla v}} + (\underline{\underline{\nabla v}})^T \right]}_{\text{High } \dot{\gamma}} + \eta_r \eta_s \left( \underline{\underline{\nabla v}} + (\underline{\underline{\nabla v}})^T \right)$$

Original Doi Theory stress equation

High  $\dot{\gamma}$

Parameters adjusted for optimal rheological data:

$$\overline{D}_r = D_r \frac{4}{9} (1 - \underline{\underline{S}} : \underline{\underline{S}})^{-2} \quad U = v_2 c d L^2 \quad \begin{array}{l} \eta_r = \text{relative viscosity} \\ \eta_s = \text{solvent/matrix viscosity} \end{array}$$

➤ Behavior of polymer melt:

➤ **Introduce modification:** Extend to non-Newtonian solvents (polymer melts)  
Introduce memory effect (viscoelasticity)

➤ Rheological models: Carreau - Yosuda Model

$$\frac{\eta_s - \eta_{s,\infty}}{\eta_{s,0} - \eta_{s,\infty}} = \left[ 1 + (\lambda I_2)^a \right]^{\frac{n-1}{a}}$$

➤ Viscoelasticity: Upper Convected Maxwell

$$\underline{\underline{\tau}} + \lambda \left[ \frac{\partial \underline{\underline{\tau}}}{\partial t} + (\underline{\underline{v}} \cdot \nabla \underline{\underline{\tau}}) - \left[ (\nabla \underline{\underline{v}})^T \cdot \underline{\underline{\tau}} + \underline{\underline{\tau}} \cdot \nabla \underline{\underline{v}} \right] \right] = \eta \dot{\underline{\underline{\gamma}}}$$

➤ Equation of Transport

$$\underline{\underline{v}} = 0$$

(Mass)

$$\underline{\underline{\sigma}} = \underline{\underline{\tau}} + p \underline{\underline{I}}$$

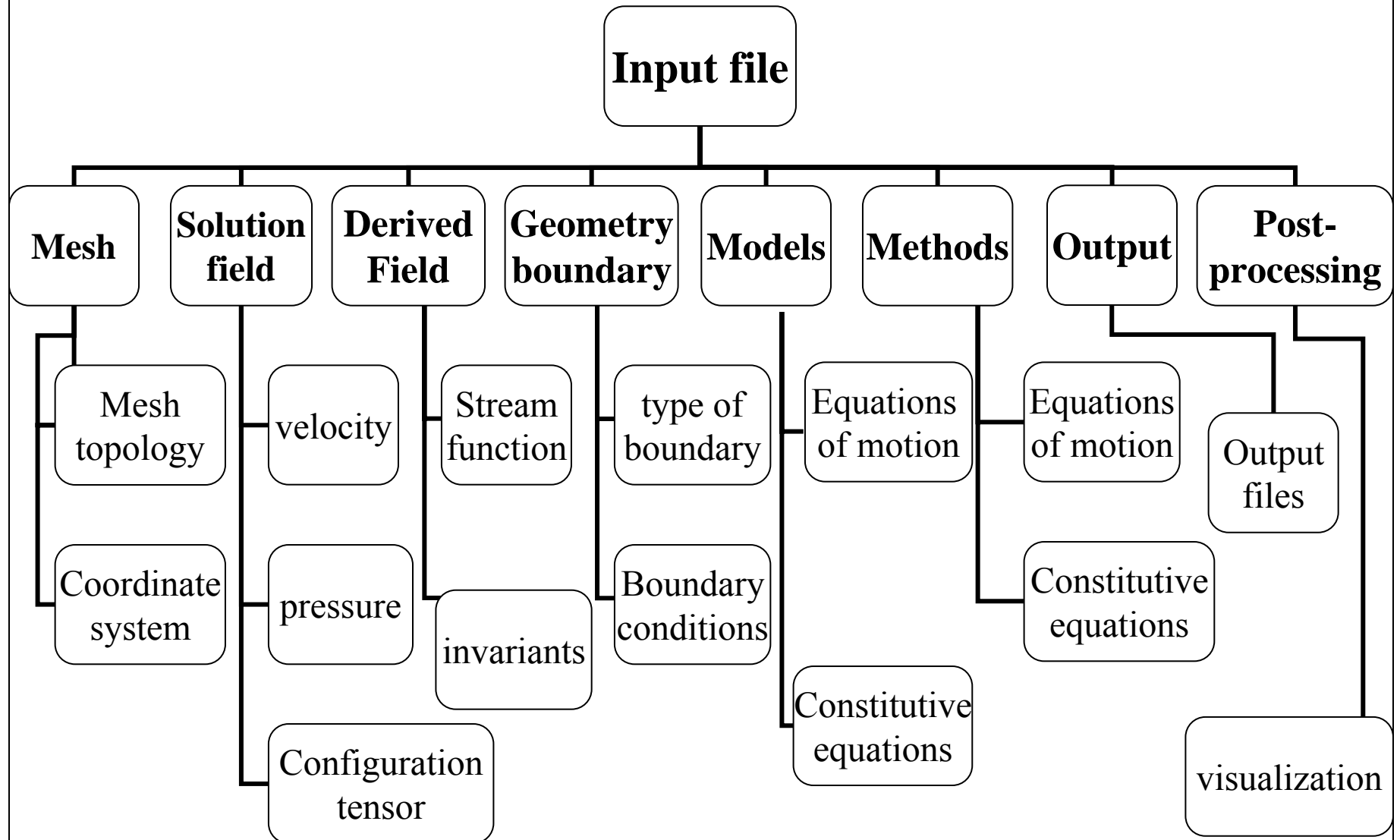
(Momentum)

$$\rho C_p \frac{DT}{Dt} = (kT_{,i})_{,i} + \underline{\underline{\tau}} \underline{\underline{D}}$$

(Energy)



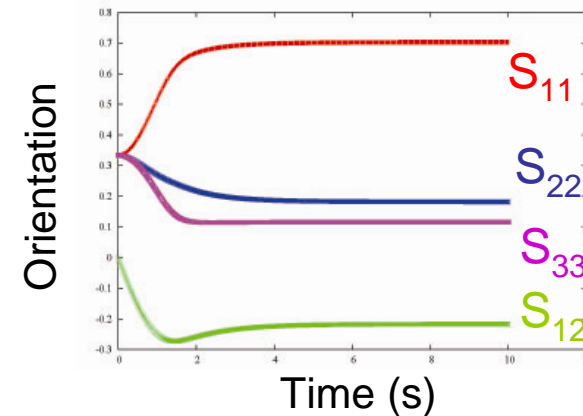
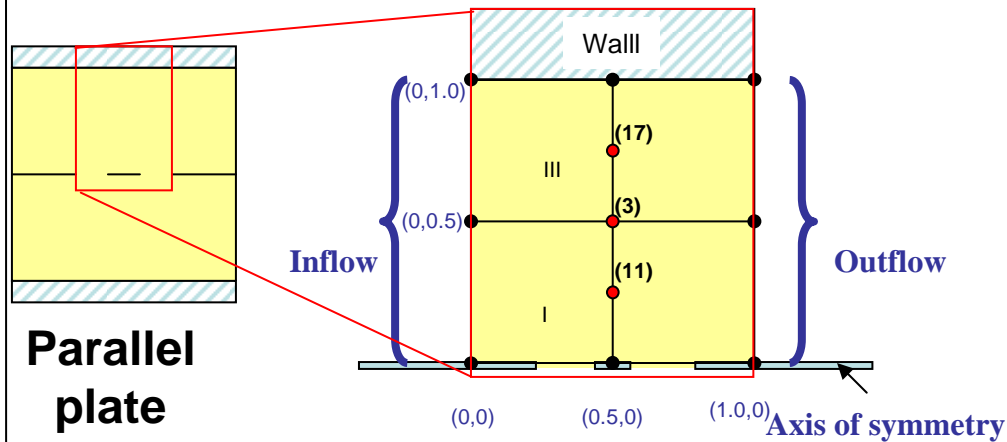
# PROGRAM STRUCTURE



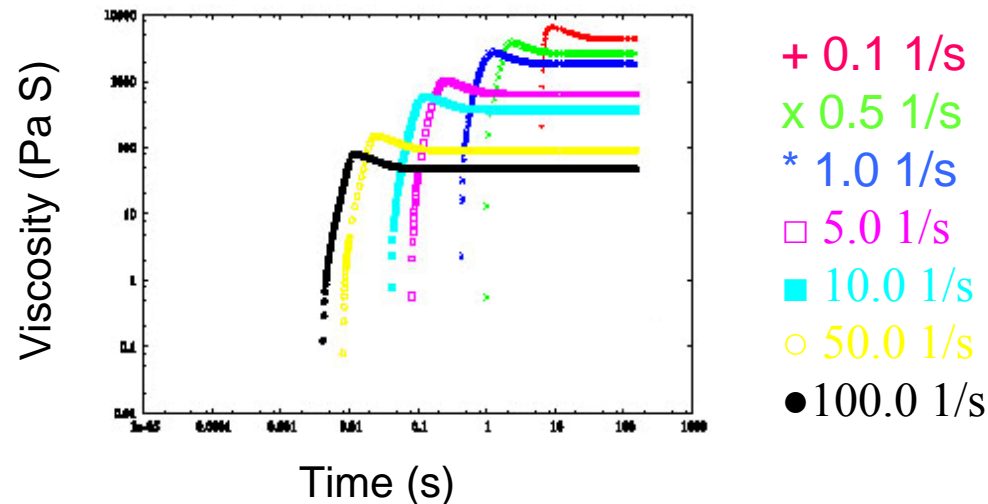
# SIMULATION SCHEME

- Determine the free surface shape
  - Mavridis technique
- Orientation tensor of fiber suspensions
  - **Discontinuous Galerkin** (DG) finite element methods have been successful for the discretization of the equations of motion when additionally a discrete elastic viscous stress splitting technique is used
  - The discretized equations can be solved element by element
- Configuration tensor of viscoelastic fluids
  - **Galerkin finite element** methods have been successful for the discretization of the equations of motion when additionally a discrete elastic viscous stress splitting technique is used
  - A frontal solver will be used to solve the matrix-vector equation resulting from the Galerkin method
- Use of two techniques recently developed to ensure positive definiteness of the configuration tensor at the discrete level
- A typical iteration step consists of three stages
  1. Update the velocity using the stresses from the previous time step
  2. Update the orientation tensor and the stress using the velocity computed in 1
  3. Update the free boundary coordinates and mesh using the velocity computed in stage 1

# NUMERICAL RESULTS



Preliminary results on model predictions of the orientation for  $S_{11}$ ,  $S_{22}$ ,  $S_{33}$ ,  $S_{12}$  components using Backward-tracking Lagrangian Method (BLPM). The model predicted orientation components, at an Node 3, for  $0 \leq t \leq 10$  s in a fluid moving between parallel plates. Similar results were obtained using a rheometrical simulation method.



The rheometrical simulations are able to predict some important viscoelastic quantities. Here is shown a representative result of the prediction of the transient viscosity at several shear rates. The constants used for the model were:  $A=0$ ,  $Dr=18,000$ ,  $G=3.2$ ,  $U=0.1$ .

# EXPERIMENTAL DETERMINATION OF FIBER ORIENTATION



Long glass fiber  
Pultruded in PP



Short shots  
progression



Short shots  
progression



Top view

Side view



Front view



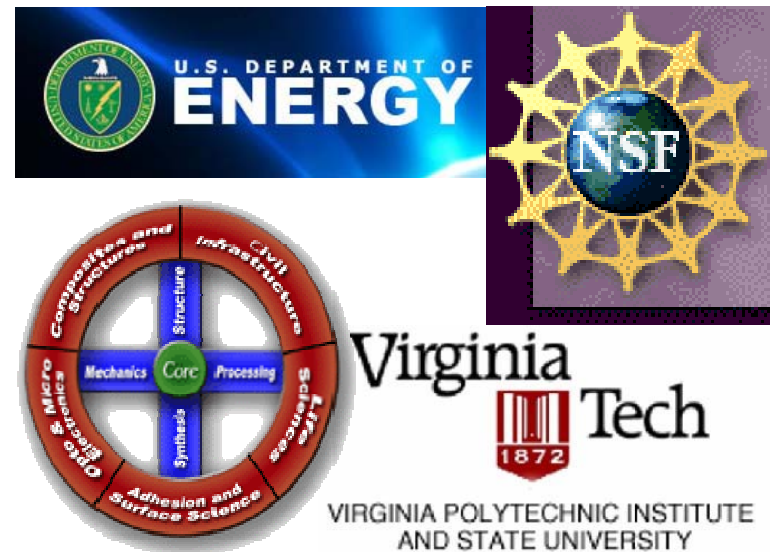
A method to determine the fiber orientation in Injection Molded part will be tried to develop during this summer in collaboration with:

# FINDINGS

- Preliminary orientations of fibers have been determined using two simulation methods: complex flow and rheometrical flow.
- Initial experiments indicate that additional modification of the theory may be necessary to simulate long fiber orientations.

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